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JOINT INSTITUTE FOR LABORATORY ASTROPHYSICS



UNIVERSITY OF COLORADO

REPORT



NATIONAL BUREAU OF STANDARDS

CLASSICAL PATH BROADENING FUNCTIONS
FOR A DEBYE-SHIELDED INTERACTION

by

J. Cooper

S. Klarsfeld

and

G. K. Oertel

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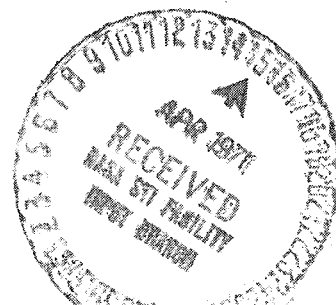
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Classical Path Broadening Functions

For a Debye-Shielded Interaction

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Abstract

Stark broadening calculations of isolated neutral atom lines in the classical path approximation usually involve an electron (moving along a straight line path) interacting directly with the atom. Correlations between the electrons are then taken into account by imposing a cutoff in the interaction, when the distance from the atom, ρ , exceeds the Debye length, ρ_D . A more consistent procedure for the correlation effects is to replace the direct interaction of the electron by a Debye-shielded interaction. The functions A, B, a and b which are required in the theory when the Debye-shielded interaction is used are considered in detail in this report. When $\rho/\rho_D < 0.1$, it is found that the a and b functions may be closely reproduced by using unshielded functions in conjunction with an upper cutoff of $0.68 \rho_D$. In the appendix is a computer program to generate these functions written by U. Palmer of JILA.

1. Introduction

Calculations of the broadening by electrons in the impact approximation usually involve the evaluation of an operator (the ϕ operator) in which the classical path S-matrices for the electron collisions have been expanded to second order (see, for example, Refs. 1, 2 and 3). Higher order terms in the expansion are then accounted for by a lower cutoff in the integral over impact parameters, and the effect of electron correlations is included by an upper cutoff at an impact parameter at the order of the Debye length. The purpose of this report is to give an alternative numerical procedure to the use of the upper cutoff (although we will show in Sec. 6 that a judicious choice of upper cutoff will, under some circumstances, reproduce our results).

More recent theory^{4,5} has shown that the broadening operator for the complete line profile which is correct to second order in the interaction potential $V(t)$ can be expressed (for $|\alpha\rangle$, $|\alpha'\rangle$ matrix elements), using Eq. (49) of Ref. 4, as

$$\langle\alpha|\mathcal{L}(\Delta\omega)|\alpha'\rangle = -i\sum_k \langle\alpha|\int_0^\infty dt e^{i\Delta\omega_k t} \{V(t)|k\rangle\langle k|V(0)\}_{Av}|\alpha'\rangle \quad (1.1)$$

Here intermediate states $|k\rangle$ have been explicitly inserted and $\Delta\omega_k$ is the frequency difference of the radiation from the intermediate state. This result was originally obtained by Baranger⁶ from a wing expansion, rather than the more complete general theory. In particular this result has important consequences, since it shows [see Eq. (1.3) below] that, in the correct second-order treatment, functions like $A(z_1, z_2)$ as introduced in Ref. 3 corresponding to off-diagonal elements of the broadening operator are needed only for the simple case of $z_1 = z_2$.

Putting the potential $V(t)$ equal to the dipole interaction $-\vec{d} \cdot \vec{E}(t)$ where $\vec{E}(t)$ is the electric field due to all the electrons, we see that Eq. (1.1) involves the evaluation of the electric field autocorrelation function, namely:

$$g(\Delta\omega) = \int_0^\infty dt e^{i\Delta\omega t} \{ \vec{E}(t) \vec{E}(0) \}_{Av} \quad (1.2)$$

This function has been examined in Refs. 7 and 8. In particular, it is possible to evaluate the electric field average as if each electron were an independent quasi-particle interacting with the radiating atom through its dynamically screened electric field. The full evaluation of the dynamically screened potential requires the use of the wave number and frequency-dependent dielectric constant $\epsilon^+(\vec{k}, \vec{k} \cdot \vec{v})$, however, the dominant contribution to $g(\Delta\omega)$ is from the region where $\Delta\omega \simeq \vec{k} \cdot \vec{v}$ [and in fact, $\vec{k} \cdot \vec{v}$ is set equal to $\Delta\omega$ for the real part of $g(\Delta\omega)$ ⁸]. In general, the full evaluation of $g(\Delta\omega)$ is quite complicated,^{8,9} but, when $\Delta\omega \ll \omega_p$ (the plasma frequency) the dynamic dielectric constant can be approximated by the static dielectric constant and the shielded field is the Debye-screened field. When $\Delta\omega \gg \omega_p$, unshielded fields must be used.

In this report, we consider the evaluation of the second-order terms using static Debye-screened fields. This is therefore only strictly correct when $\Delta\omega$ (the frequency separation to the intermediate state) is less than ω_p ; however, correlation and shielding are most important in this region where the lines of the spectrum are overlapping or starting to overlap. In addition, when $\Delta\omega \gg \omega_p$ the difference between using static Debye-screened fields and unshielded fields in Eq. (1.2) is negligible, and the value of Eq. (1.2) is quite small in any case. Finally, by comparison with the re-

sults of Ref. 8 [in particular for the real part of $g(\Delta\omega)$] errors in the region $\Delta\omega \simeq \omega_p$ from the use of Debye-screened fields are not expected to be large, provided $g(\Delta\omega)$ is not appreciably enhanced in this region due to instabilities and other non-thermal effects.

To relate Eq. (1.2) to the usual A and B functions, it is necessary to rewrite it slightly. Since the electrons act as independent quasi-particles the average in Eq. (1.2) may be written in terms of integrals over the frequency of collisions dv (an integral essentially over velocities and impact parameters) and the time of closest approach t_0 (see for example section 4B of Ref. 4 and Ref. 10).

Thus

$$\begin{aligned}
 & \int_0^\infty e^{i\Delta\omega t} \{ \vec{E}(t) \vec{E}(0) \}_{Av} dt \\
 &= \int_{-\infty}^\infty dt_0 \int dv \int_0^\infty dt e^{i\Delta\omega t} \vec{E}_s(t+t_0) \vec{E}_s(t_0) \quad \text{where } \vec{E}_s \text{ represents the} \\
 & \quad \text{shielded field}^8 \\
 &= \int dv \int_{-\infty}^\infty dx_2 \int_{x_2}^\infty dx_1 e^{i\Delta\omega(x_1-x_2)} \vec{E}_s(x_1) \vec{E}_s(x_2) \quad \text{with } \begin{matrix} x_1=t+t_0 \\ x_2=t_0 \end{matrix} \\
 &= \int dv \int_{-\infty}^\infty dx_1 \int_{-\infty}^{x_1} dx_2 e^{i\Delta\omega(x_1-x_2)} \vec{E}_s(x_1) \vec{E}_s(x_2) \tag{1.3}
 \end{aligned}$$

by using the Dirichlet integral formula [see Eq. (57), Ref. 4].

2. The Shielded Broadening Functions

Thus, using static Debye-screened fields instead of pure Coulomb fields, which amounts to multiplying the latter by $(1+r/\rho_D)\exp(-r/\rho_D)$, the usual second-order time integral¹⁻³ is replaced by

$$F(z, z'; q) = A + iB =$$

$$= \frac{1}{2} \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dx' (1+xx') g(x; q) g(x'; q) e^{i(zx - z'x')} \quad , \quad (2.1)$$

where

$$g(x; q) = \left[1 + q(1+x^2)^{1/2} \right] (1+x^2)^{-3/2} e^{-q(1+x^2)^{1/2}} \quad , \quad (2.2)$$

$z = \rho\omega/v$, $z' = \rho\omega'/v$, $q = \rho/\rho_D$, ρ is the impact parameter, $\rho_D = (kT/4\pi Ne^2)^{1/2}$ the Debye length, and v the electron velocity. It is easily seen that the new A and B functions possess the same symmetry properties as the unshielded ones, viz.³

$$A(z, z'; q) = A(z', z; q) = A(-z, -z'; q) \quad , \quad (2.3)$$

$$B(z, z'; q) = B(z', z; q) = -B(-z, -z'; q) \quad . \quad (2.4)$$

The general expression in Eq. (2.1) should be used in the impact theory^{1,3} to compute the matrix elements of the broadening operator for lines with forbidden components (for an isolated line $z' = z$). However, as stressed earlier, in the unified theory approach only "diagonal" functions with $z = z' = \rho\Delta\omega_k/v$ will occur. Of course, no upper cutoff on impact parameters is required with the new functions.

Sticking to real integration variables in Eq. (2.1), simple parity considerations show that the A-function is given by

$$A = \int_0^{\infty} dx g(x; q) \cos(zx) \int_0^{\infty} dx' g(x'; q) \cos(z'x') \\ + \int_0^{\infty} dx x g(x; q) \sin(zx) \int_0^{\infty} dx' x' g(x'; q) \sin(z'x') \quad . \quad (2.5)$$

The necessary Fourier transforms are readily obtained from¹¹

$$\int_0^{\infty} dx (\alpha^2 + x^2)^{-1/2} e^{-q(\alpha^2 + x^2)^{1/2}} \cos(zx) = K_0[\alpha(z^2 + q^2)^{1/2}] \quad , \quad (2.6)$$

$$\int_0^\infty dx x(\alpha^2+x^2)^{-1/2} e^{-q(\alpha^2+x^2)^{1/2}} \sin(zx) = \alpha z (z^2+q^2)^{-1/2} K_1[\alpha(z^2+q^2)^{1/2}], \quad (2.7)$$

by differentiation with respect to α . Here K_0 and K_1 are modified Bessel functions of the second kind. Hence:

$$A(z, z'; q) = zz' K_0(R) K_0(R') + RR' K_1(R) K_1(R') \quad , \quad (2.8)$$

where we have put for brevity

$$R = (z^2+q^2)^{1/2}, \quad R' = (z'^2+q^2)^{1/2} \quad . \quad (2.9)$$

For the diagonal function we get

$$A(z, z; q) \equiv A(z; q) = z^2 K_0^2(R) + R^2 K_1^2(R) \quad (2.10)$$

Since z , z' , and q are all proportional to ρ , the integration over the impact parameter (now from ρ_{\min} to ∞) can be expressed in terms of

$$a(z, z'; q) = \int_1^\infty \frac{d\lambda}{\lambda} A(\lambda z, \lambda z'; \lambda q) \quad , \quad (2.11)$$

which represents the natural generalization of the function $a(z)$ of GBK0.

To save space, we give here the results only for the case $z = z'$:

$$a(z; q) = RK_0(R)K_1(R) - \frac{1}{2}q^2[K_1^2(R) - K_0^2(R)] \quad (2.12)$$

It is also convenient to introduce in Eqs. (2.10), (2.12), a new parameter $z_D = z/q = \rho_D \Delta\omega/v$, so that $R = \beta z$, with $\beta = (1+1/z_D^2)^{1/2}$. For $z_D \sim \Delta\omega/\omega_p \gg 1$ one has $A(z; z/z_D) \cong A(z)$ and $a(z; z/z_D) \cong a(z)$. Therefore, when $\Delta\omega \gg \omega_p$, using either shielded fields or unshielded fields in Eq. (1.2) gives the same results. As we have said before, the fact that we get the correct answer in the important limit of $\Delta\omega \ll \omega_p$ and that both shielded and unshielded fields give nearly identical results when $\Delta\omega \gg \omega_p$ is the main justification for the functions presented here.

3. Dispersion Relations for Off-Diagonal Broadening Functions

A convenient way to calculate the B function, once A is known, is provided by the dispersion relation, which expresses B as a Hilbert transform of A. This method has been extensively used in the past to compute various diagonal B functions contributing to the broadening of isolated lines emitted by neutral atoms and positive ions.^{1,12-14} In both cases the dispersion relations merely reflect the analyticity of the second-order time integral with respect to one of its parameters, considered as a complex variable.

The extension to off-diagonal functions must be done with some care. In this case it is better to introduce an auxiliary complex variable, while keeping all physical parameters real (the dispersion relations given recently¹⁵ for the neutral functions $A(z, pz)$ and $B(z, pz)$, where $p = z'/z$ is a real fixed ratio, are wrong, since for $p \neq 1$ the time integral does not possess the required analytic properties when z is allowed to take complex values). For instance, from the structure of Eq. (2.1):

$$F(z, z'; q) = \int_{-\infty}^{\infty} dx \int_{-\infty}^x dx' f(x, x'; q) e^{i(zx - z'x')} \quad , \quad (3.1)$$

it is apparent that for any real z , z' , and $q \geq 0$, the function $\varphi(\zeta) = F(z + \zeta, z' + \zeta; q)$ is holomorphic in the upper half-plane $\text{Im}\zeta > 0$. Applying the usual analysis, based upon Cauchy's theorem and the well-known relation $1/(\zeta - i0) = P(1/\zeta) + i\pi\delta(\zeta)$, one readily gets

$$\varphi(0) = \frac{1}{\pi i} P \int_{-\infty}^{\infty} d\zeta \frac{\varphi(\zeta)}{\zeta} \quad , \quad (3.2)$$

whence

$$B(z, z'; q) = -\frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{d\zeta}{\zeta} A(z+\zeta, z'+\zeta; q) \quad , \quad (3.3)$$

or alternatively

$$B(z, z'; q) = -\frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{d\zeta}{\zeta - \frac{1}{2}(z+z')} A[\zeta + \frac{1}{2}(z-z'), \zeta - \frac{1}{2}(z-z'); q] \quad . \quad (3.4)$$

Notice that Eq. (3.3) can be given also the equivalent form

$$B(z, z'; q) = -\frac{1}{\pi} \int_0^{\infty} \frac{d\zeta}{\zeta} [A(z+\zeta, z'+\zeta; q) - A(z-\zeta, z'-\zeta; q)] \quad (3.5)$$

from which the singularity has been removed.

Although the above relations allow us in principle to compute B to the desired accuracy, in practice the limiting process inherent to all of them might become sometimes a serious source of trouble.

4. Complex Integration

We shall now apply to the shielded case the powerful contour integration method which led to closed-form expressions for both A and B in the non-shielding limit $q = 0$.¹⁶ To this end we assume $z \geq z' > 0$, and make the change of variables $x = \sinh u$, $x' = \sinh u'$. Equation (2.1) may then be rewritten as

$$F = F_1(z, z'; q) + F_2(z, z'; q) \quad , \quad (4.1)$$

where

$$F_1 = \frac{1}{2} \int_{-\infty}^{\infty} du \sinh u \frac{1+q \cosh u}{\cosh^2 u} e^{-q \cosh u + iz \sinh u} \phi_1(u), \quad (4.2)$$

with

$$\phi_1(u) = \int_{-\infty}^u du' \sinh u' \frac{1+q \cosh u'}{\cosh^2 u'} e^{-q \cosh u' - iz' \sinh u'} , \quad (4.3)$$

and

$$F_2 = \frac{1}{2} \int_{-\infty}^{\infty} du \frac{1+q \cosh u}{\cosh^2 u} e^{-q \cosh u + iz \sinh u} \phi_2(u) , \quad (4.4)$$

with

$$\phi_2(u) = \int_{-\infty}^u du' \frac{1+q \cosh u'}{\cosh^2 u'} e^{-q \cosh u' - iz' \sinh u'} . \quad (4.5)$$

Let us first evaluate F_1 . Since

$$\sinh x \frac{1+q \cosh x}{\cosh^2 x} e^{-q \cosh x} = - \frac{d}{dx} \left(\frac{e^{-q \cosh x}}{\cosh x} \right) , \quad (4.6)$$

integration by parts gives

$$\phi_1(u) = -(1/\cosh u) e^{-q \cosh u - iz' \sinh u} - iz' \psi_1(u) , \quad (4.7)$$

where

$$\psi_1(u) = \int_{-\infty}^u du' e^{-q \cosh u' - iz' \sinh u'} , \quad (4.8)$$

and further

$$\begin{aligned} 2F_1 = & - \int_{-\infty}^{\infty} du \sinh u \frac{1+q \cosh u}{\cosh^3 u} e^{-2q \cosh u + i\eta \sinh u} \\ & - iz' \int_{-\infty}^{\infty} (du/\cosh u) e^{-2q \cosh u + i\eta \sinh u} + zz' G_1 , \end{aligned} \quad (4.9)$$

where $\eta = z-z' \geq 0$, and

$$G_1 = \int_{-\infty}^{\infty} du e^{-q \cosh u + iz \sinh u} \int_{-\infty}^u du' e^{-q \cosh u' - iz' \sinh u'} . \quad (4.10)$$

Defining

$$\tan \alpha = q/z, \quad \tan \alpha' = q/z', \quad (0 \leq \alpha \leq \alpha' \leq \pi/2) \quad , \quad (4.11)$$

we may rewrite G_1 as

$$G_1 = \int_{-\infty}^{\infty} du \, e^{iR \sinh(u+i\alpha)} \int_{-\infty}^u du' \, e^{-iR' \sinh(u'-i\alpha')} \quad (4.12)$$

with R, R' given by Eq. (2.9) and $R \geq R'$.

We now consider u and u' as complex variables and transform Eq. (4.12) into a repeated contour integral $G_1 = \int_{\Gamma} du \dots \int_{\Gamma_u} du' \dots$, with the contours shown in Fig. 1. It is easily seen that the contribution of the

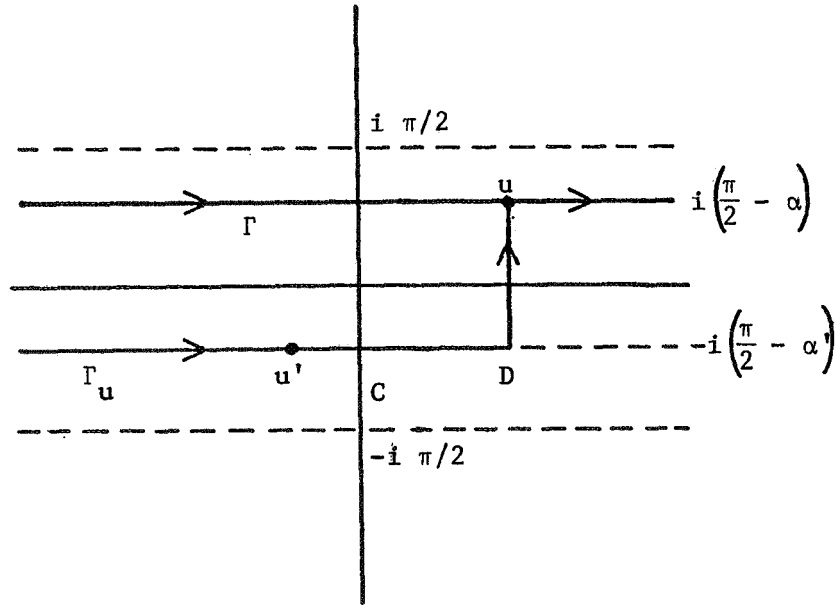


Figure 1

segment CD vanishes, since $\int_0^u du' \dots$ is an odd function of u , and therefore

$$G_1 = \int_{-\infty}^{\infty} du e^{-R \cosh u} \left[\int_{-\infty}^0 du' e^{-R' \cosh u'} + i \int_0^{\pi-\alpha-\alpha'} d\theta e^{-R' \cosh(u+i\theta)} \right] =$$

$$= 2 K_0(R) K_0(R') + i M_1, \quad (4.13)$$

where

$$M_1 = \int_0^{\pi-\alpha-\alpha'} d\theta \int_{-\infty}^{\infty} du e^{-R \cosh u - R' \cosh(u+i\theta)}. \quad (4.14)$$

After shifting the u integration from the real axis onto the line $\text{Im } u = -\chi(u \rightarrow u-i\chi)$, with χ given by $\tan \chi = R' \sin \theta / (R + R' \cos \theta) > 0$, and changing θ in $\pi - 2\theta$, one gets

$$M_1 = 4 \int_{(\alpha+\alpha')/2}^{\pi/2} d\theta K_0[S(\theta)], \quad (4.15)$$

where

$$S(\theta) = (R^2 + R'^2 - 2RR' \cos 2\theta)^{1/2}. \quad (4.16)$$

The second term F_2 in Eq. (4.1) can be treated in a similar manner, but the calculation is slightly more cumbersome. Starting from

$$\frac{1+q \cosh x}{\cosh^2 x} e^{-q \cosh x} = \frac{d}{dx} \left(\frac{\sinh x}{\cosh x} e^{-q \cosh x} \right) + q \cosh x e^{-q \cosh x}, \quad (4.17)$$

one first obtains by partial integration

$$2F_2 = \int_{-\infty}^{\infty} du \sinh u \frac{1+q \cosh u}{\cosh^3 u} e^{-2q \cosh u + i\eta \sinh u} \\ - \int_{-\infty}^{\infty} du \tanh u (q \cosh u + iz' \sinh u) e^{-2q \cosh u + i\eta \sinh u} + RR' G_2, \quad (4.18)$$

where

$$G_2 = \int_{-\infty}^{\infty} du \sinh(u+i\alpha) e^{iR \sinh(u+i\alpha)} \int_{-\infty}^u du' \sinh(u'-i\alpha') e^{-iR' \sinh(u'-i\alpha')}. \quad (4.19)$$

By contour integration this can be reduced further to

$$G_2 = 2 K_1(R) K_1(R') + i \pi, \quad (4.20)$$

where

$$M_2 = 4 \int_{(\alpha+\alpha')/2}^{\pi/2} d\theta \sin^2 \theta K_0(S) + 4 \int_{(\alpha+\alpha')/2}^{\pi/2} d\theta K_1(S)/S \\ - 4(R-R')^2 \int_{(\alpha+\alpha')/2}^{\pi/2} d\theta \cos^2 \theta K_2(S)/S^2. \quad (4.21)$$

With F_1 determined from Eqs. (4.9), (4.13) and (4.15), and F_2 from Eqs. (4.18), (4.20) and (4.21), we go back to Eq. (4.1) and separate the real and imaginary parts of F . This yields for A the closed form expression already found in Sec. 2:

$$A(z, z'; q) = z z' K_0(R) K_0(R') + R R' K_1(R) K_1(R'), \quad (4.22)$$

and for B the integral representation

$$\begin{aligned}
 B(z, z'; q) = & -q(z+z')K_1(S_0)/S_0 + 2zz' \int_{(\alpha+\alpha')/2}^{\pi/2} d\theta K_0(S) \\
 & + 2RR' \int_{(\alpha+\alpha')/2}^{\pi/2} d\theta \sin^2 \theta K_0(S) + 2RR' \int_{(\alpha+\alpha')/2}^{\pi/2} d\theta K_1(S)/S \\
 & - 2RR'(R-R')^2 \int_{(\alpha+\alpha')/2}^{\pi/2} d\theta \cos^2 \theta K_2(S)/S^2, \quad (4.23)
 \end{aligned}$$

where $S_0 = (\eta^2 + 4q^2)^{1/2}$, and S is given by Eq. (4.16).

The above form of B is not quite satisfactory for numerical computation, since it contains terms which diverge individually under certain circumstances, although the net result will always be finite (for instance, in the diagonal case $z'=z$ the first term behaves like $1/q$ when $q \rightarrow 0$, and so does the fourth). This difficulty is, however, easily resolved by noticing that S_0 is nothing but the value of S at the lower limit of integration $\theta = \frac{1}{2}(\alpha+\alpha')$. Developing the right-hand side of the identity

$$-q(z+z')K_1(S_0)/S_0 = RR' \int_{(\alpha+\alpha')/2}^{\pi/2} d \left[\sin 2\theta K_1(S)/S \right] \quad (4.24)$$

and substituting into Eq. (4.23) then enables us to eliminate the unpleasant terms and eventually results in the new integral representation

$$B(z, z'; q) = 2zz' \int_{(\alpha+\alpha')/2}^{\pi/2} d\theta K_0(S) - 2RR' \int_{(\alpha+\alpha')/2}^{\pi/2} d\theta \cos 2\theta K_0(S), \quad (4.25)$$

which is the best we can get.

In view of the subsequent integration over the impact parameter we define, by analogy with Eq. (2.11), the function

$$b(z, z'; q) = \int_1^\infty \frac{d\lambda}{\lambda} B(\lambda z, \lambda z'; \lambda q) \quad , \quad (4.26)$$

which generalizes the function $b(z)$ of GBK0. Substituting from Eq. (4.25) and noticing that α and α' do not depend on λ , one readily gets

$$b(z, z'; q) = 2zz' \int_{(\alpha+\alpha')/2}^{\pi/2} d\theta K_1(S)/S - 2RR' \int_{(\alpha+\alpha')/2}^{\pi/2} d\theta \cos 2\theta K_1(S)/S \quad . \quad (4.27)$$

In the diagonal case, Eqs. (4.25) and (4.27) simplify respectively to

$$B(z; q) = 2z^2 \int_\alpha^{\pi/2} d\theta K_0(2R \sin \theta) - 2R^2 \int_\alpha^{\pi/2} d\theta \cos 2\theta K_0(2R \sin \theta) \quad , \quad (4.28)$$

and

$$b(z; q) = (z^2/R) \int_\alpha^{\pi/2} d\theta K_1(2R \sin \theta)/\sin \theta - R \int_\alpha^{\pi/2} d\theta \cos 2\theta K_1(2R \sin \theta)/\sin \theta \quad . \quad (4.29)$$

If we let here $q \rightarrow 0$ we obtain compact integral representations for the unshielded shift functions, viz.

$$B(z) = 4z^2 \int_0^{\pi/2} d\theta \sin^2 \theta K_0(2z \sin \theta) \quad , \quad (4.30)$$

$$b(z) = 2z \int_0^{\pi/2} d\theta \sin \theta K_1(2z \sin \theta) \quad . \quad (4.31)$$

The connection with the closed form expressions reported earlier¹⁶ is provided by Nicholson's formula¹⁷

$$I_n(z) K_\nu(z) = (-)^n (2/\pi) \int_0^{\pi/2} d\theta \cos(n+\nu)\theta K_{\nu-n}(2z \cos \theta) \quad , \quad (4.32)$$

valid when n is an integer, and $|\operatorname{Re}(v-n)| < 1$. Corresponding results are not likely to hold for the shielded functions, which are represented by incomplete integrals with a variable limit. However, the latter are much easier to handle numerically than the principal value integrals in Sec. 3.

5. Approximate formulae

In this section we collect various useful approximate expressions of the shielded broadening functions, restricting ourselves to the "diagonal" case, which is the most important in practice.

We begin with asymptotic formulae for A and a , valid when z or/and q are large. These are obtained simply by substituting the standard expansions of K_0 and K_1 ¹⁸ into Eqs. (2.10) and (2.12). The leading terms are respectively

$$A(z;q) \sim (\pi/2)(1+z^2/R^2) R e^{-2R}, \quad (5.1)$$

$$a(z;q) \sim (\pi/2)(1-q^2/2R^2) e^{-2R}. \quad (5.2)$$

In particular, if one is interested in the asymptotic behavior for $\rho \rightarrow \infty$, then one must let both z and q tend to infinity, while keeping their ratio $z/q = z_D$ finite. Thus, when $z \rightarrow \infty$:

$$A(z;z/z_D) \sim (\pi/2)(\beta+1/\beta) z e^{-2\beta z}, \quad (5.3)$$

$$a(z;z/z_D) \sim (\pi/2\beta)(\beta+1/\beta) e^{-2\beta z}, \quad (5.4)$$

where $\beta = (1+1/z_D^2)^{1/2}$.

On the other hand, for $\rho \rightarrow 0$ one has

$$a(z;z/z_D) \simeq \log(0.68z_D/z), \quad \text{for } z_D \ll 1, \quad (5.5)$$

whereas $A(z; z/z_D) \rightarrow 1$.

The corresponding formulas for B and b may be derived from the integral representations given in Sec. 4. Let us assume first that only $z \rightarrow \infty$, while q remains finite. After changing the variable in Eq. (4.29) to $u = 2 R \sin \theta$, we expand it as follows:

$$\begin{aligned} B = & \frac{z^2 - R^2}{R} \int_{2q}^{2R} du K_0(u) + \frac{3R^2 + z^2}{8R^3} \int_{2q}^{2R} du u^2 K_0(u) \\ & + \frac{5R^2 + 3z^2}{128R^5} \int_{2q}^{2R} du u^4 K_0(u) + \dots \end{aligned} \quad (5.6)$$

This is readily transformed into an asymptotic expansion by developing the coefficients in powers of $1/z$ and extending all the integrations to infinity. Eventually

$$B(z; q) \sim C_1(q)/z + C_3(q)/z^3 + \dots, \quad z \rightarrow \infty \quad (5.7)$$

where

$$\begin{aligned} C_1(q) = & \left(\frac{1}{2} - q^2 \right) Ki_1(2q) + 2q^2 K_1(2q) + qK_0(2q), \\ C_3(q) = & \left(\frac{9}{16} - \frac{3q^2}{8} + \frac{q^4}{2} \right) Ki_1(2q) + \left(\frac{9}{4} - \frac{q^2}{2} \right) q^2 K_1(2q) \\ & + \left(\frac{9}{8} + \frac{3q^2}{4} \right) qK_0(2q), \end{aligned} \quad (5.8)$$

with the new function Ki_1 defined by¹⁸

$$Ki_1(x) = \int_x^\infty du K_0(u). \quad (5.9)$$

Since $Ki_1(0) = \pi/2$, in the limit $q \rightarrow 0$ one has $C_1(0) = \pi/4$, $C_3(0) = 9\pi/32$, and we recover the well-known asymptotic expansion of B(z).

Similarly, from Eq. (4.29) one obtains

$$b(z;q) \sim c_1(q)/z + c_3(q)/z^3 + \dots, \quad z \rightarrow \infty \quad (5.10)$$

where

$$\begin{aligned} c_1(q) &= \left(\frac{1}{2} + q^2\right) Ki_1(2q) - q^2 K_1(2q) + q K_0(2q), \\ c_3(q) &= \left(\frac{3}{16} - \frac{3q^2}{8} - \frac{q^4}{2}\right) Ki_1(2q) + \left(\frac{3}{4} + \frac{q^2}{2}\right) q^2 K_1(2q) \\ &\quad + \left(\frac{3}{8} - \frac{q^2}{4}\right) q K_0(2q) \end{aligned} \quad (5.11)$$

In the limit $q \rightarrow 0$ we have $c_1(0) = \pi/4$, $c_3(0) = 3\pi/32$, and Eq. (5.10) reduces to the asymptotic expansion of $b(z)$.

The above procedure clearly breaks down when $q \rightarrow \infty$, since all the terms in Eq. (5.6) are then of the same order. If z is kept finite an asymptotic estimate of B is, however, readily obtained from Eq. (4.28) by noticing that the integration interval shrinks as q is increased ($\pi/2 - \alpha \sim z/q$). This allows us to write

$$\begin{aligned} B(z;q) &\sim (2z^2 - 2R^2 \cos 2\alpha) K_0(2R \sin \alpha) (\pi/2 - \alpha) \\ &\sim 2zq K_0(2q), \quad q \rightarrow \infty. \end{aligned} \quad (5.12)$$

Similarly, from Eq. (4.30) we get

$$b(z;q) \sim z K_1(2q), \quad q \rightarrow \infty. \quad (5.13)$$

Hence, when $z \ll q$ both B and b become exponentially small and depend linearly on z .

Let us consider now the case when z and q tend together to infinity so

that their ratio $z/q = z_D$ remains finite. In this case no shrinkage occurs, but the integrals in Eqs. (4.28) and (4.29) may be evaluated asymptotically on integrating by parts.¹⁹ Neglecting higher order contributions one finds

$$B(z; z/z_D) \sim (z/z_D)^2 K_1(2z/z_D), \quad z \rightarrow \infty \quad (5.14)$$

and

$$b(z; z/z_D) \sim (1/2z_D) K_0(2z/z_D), \quad z \rightarrow \infty \quad (5.15)$$

At the opposite limit, as $\rho \rightarrow 0$, from Eq. (4.28) one gets $B(z; z/z_D) \rightarrow 0$ and Eq. (4.29) yields

$$b(z; z/z_D) \rightarrow \arctan z_D - \frac{1}{2} z_D / (1 + z_D^2), \quad z \rightarrow 0 \quad (5.16)$$

The last limit is $\cong \pi/2$ for $z_D \gg 1$, and $\cong z_D/2$ for $z_D \ll 1$.

6. Numerical results

Numerical results are not presented here in tabular form for $A(z, q)$ and $a(z, z_D)$ since the Bessel functions on Eqs. (2.10) and (2.12) are so simple to calculate (see Ref. 18, formulae 9.8.5, 9.8.6, 9.8.7 and 9.8.8). Tables 1 and 2 show calculated values of $B(z, q)$ and $b(z, z_D)$. Where asymptotic forms could not be used, these functions were calculated both from the formulae of Eqs. (4.28) and (4.29) and from the Hilbert transform Eq. (3.5) [with direct integration of Eq. (4.26) to give $b(z, z_D)$]. The first procedure was by far the simpler, however, overall agreement between the two methods of better than 2% was obtained. For values of z greater than those in the table, sufficient accuracy can be obtained by using the first terms of Eqs. (5.7) and (5.10). Notice that $B(z, q=0) = \pi z^2 [K_0(z)I_0(z) - K_1(z)I_1(z)]$ and $b(z, z_D=\infty) = \pi/2 - \pi z K_0(z)I_1(z)$ are the straight line

results. $B(z, q > 10)$ and $b(z, z_D < .002)$ are for all effective purposes negligible.

$A(z, q)$, $B(z, q)$ and $b(z, q)$ are plotted in Figs. 2, 3 and 4 for various values of $q (= \rho/\rho_D = z/z_D)$; $a(z, q)$ was not plotted, but it diverges logarithmically at small z and q [Eq. (5.5)]. Notice in particular that the functions get small rapidly when $q > 1$. This is expected since Eqs. (5.1) (5.2) (5.12) and (5.13) all predict an exponential fall off when $q \gg 1$. This rapid cutoff when $\rho \gtrsim \rho_D$, certainly to some extent justifies the usual procedure^{2,12} for treating shielding by a cutoff. To further test the validity of these cutoff procedures, in Fig. 5 a function $F(z, q)$ is plotted. $F(z, q)$ is essentially¹² $[b(z) - b(z_{\max})]$ where $z_{\max} = \rho_{\max} \omega/v$. Two cases are considered, firstly $\rho_{\max} = \rho_D$ and secondly $\rho_{\max} = 0.68 \rho_D$. In both cases the agreement between $F(z, q)$ and $b(z, q)$ of Fig. 4 is surprisingly good. (Notice, however, that $F(z, q) = 0$ for $\rho \geq \rho_{\max}$.) In fact, when $\rho/\rho_D < 0.1$ the agreement for the $\rho_{\max} = 0.68 \rho_D$ case is better than 5%. This value ($0.68 \rho_D$) was chosen as the cutoff since its use in $[a(z) - a(z_{\max})]$ exactly reproduces $a(z, z_D)$ for small z and z_D [see Eq. (5.5)], as has been noted in Ref. 7. Actually, for $q = \rho/\rho_D < 0.1$ the agreement for all values of z between $[a(z) - a(z_{\max})]$ and $a(z, z_D)$ is again always better than about 4%; and for $q < 0.1$ for both $B(z, q)$ and $A(z, q)$ the difference between these functions and the unshielded ones ($q = 0$) is also very small (see Figs. 2 and 3). We therefore conclude that the usual cutoff procedures should certainly be adequate when simplicity is desired and when $\rho/\rho_D < 0.1$ (which is true in most cases of physical interest). However, we believe that the functions presented here are of even greater utility, especially if ρ/ρ_D should get large.

TABLE 1

 $B(z, q)$

$z \backslash q$.00	.01	.10	.20	.50	1.00	2.00	5.00	10.00
.001	2.063E-05	8.165E-05	3.507E-04	4.459E-04	4.210E-04	2.278E-04	4.464E-05	1.778E-07	1.148E-11
.002	7.327E-05	1.670E-04	7.013E-04	8.917E-04	8.421E-04	4.556E-04	8.928E-05	3.556E-07	2.296E-11
.003	1.534E-04	2.609E-04	1.052E-03	1.338E-03	1.263E-03	6.834E-04	1.339E-04	5.334E-07	3.445E-11
.004	2.582E-04	3.666E-04	1.404E-03	1.784E-03	1.684E-03	9.112E-04	1.786E-04	7.112E-07	4.593E-11
.005	3.860E-04	4.866E-04	1.756E-03	2.230E-03	2.105E-03	1.139E-03	2.232E-04	8.890E-07	5.741E-11
.006	5.352E-04	6.227E-04	2.109E-03	2.677E-03	2.526E-03	1.367E-03	2.678E-04	1.067E-06	6.889E-11
.007	7.047E-04	7.761E-04	2.464E-03	3.124E-03	2.947E-03	1.595E-03	3.125E-04	1.245E-06	8.038E-11
.008	8.936E-04	9.474E-04	2.819E-03	3.571E-03	3.369E-03	1.822E-03	3.571E-04	1.422E-06	9.186E-11
.009	1.101E-03	1.137E-03	3.176E-03	4.018E-03	3.790E-03	2.050E-03	4.017E-04	1.600E-06	1.033E-10
.010	1.326E-03	1.344E-03	3.534E-03	4.466E-03	4.211E-03	2.278E-03	4.464E-04	1.778E-06	1.148E-10
.050	2.056E-02	2.034E-02	2.067E-02	2.328E-02	2.116E-02	1.139E-02	2.231E-03	8.888E-06	5.740E-10
.100	6.094E-02	6.068E-02	5.370E-02	5.156E-02	4.294E-02	2.282E-02	4.458E-03	1.776E-05	1.148E-09
.200	1.621E-01	1.619E-01	1.467E-01	1.274E-01	9.003E-02	4.584E-02	8.883E-03	3.542E-05	2.291E-09
.400	3.588E-01	3.586E-01	3.402E-01	3.029E-01	1.965E-01	9.236E-02	1.749E-02	6.999E-05	4.550E-09
.600	4.981E-01	4.978E-01	4.805E-01	4.407E-01	2.972E-01	1.369E-01	2.552E-02	1.029E-04	6.747E-09
.800	5.759E-01	5.758E-01	5.603E-01	5.230E-01	3.707E-01	1.747E-01	3.264E-02	1.335E-04	8.851E-09
1.000	6.059E-01	6.058E-01	5.922E-01	5.587E-01	4.122E-01	2.022E-01	3.854E-02	1.610E-04	1.084E-08
1.200	6.031E-01	6.030E-01	5.912E-01	5.615E-01	4.268E-01	2.183E-01	4.302E-02	1.851E-04	1.268E-08
1.400	5.801E-01	5.799E-01	5.696E-01	5.436E-01	4.221E-01	2.242E-01	4.599E-02	2.053E-04	1.436E-08
1.600	5.459E-01	5.458E-01	5.367E-01	5.136E-01	4.052E-01	2.221E-01	4.753E-02	2.215E-04	1.586E-08
1.800	5.068E-01	5.067E-01	4.987E-01	4.782E-01	3.815E-01	2.144E-01	4.780E-02	2.337E-04	1.718E-08
2.000	4.669E-01	4.668E-01	4.596E-01	4.414E-01	3.548E-01	2.033E-01	4.704E-02	2.419E-04	1.830E-08
3.000	3.054E-01	3.054E-01	3.008E-01	2.893E-01	2.353E-01	1.402E-01	3.621E-02	2.361E-04	2.105E-08
4.000	2.158E-01	2.158E-01	2.124E-01	2.041E-01	1.654E-01	9.828E-02	2.580E-02	1.916E-04	2.003E-08
5.000	1.663E-01	1.662E-01	1.636E-01	1.570E-01	1.267E-01	7.471E-02	1.938E-02	1.476E-04	1.719E-08
6.000	1.358E-01	1.358E-01	1.336E-01	1.282E-01	1.032E-01	6.051E-02	1.552E-02	1.161E-04	1.412E-08
8.000	1.001E-01	1.000E-01	9.842E-02	9.439E-02	7.582E-02	4.427E-02	1.123E-02	8.097E-05	9.683E-09
10.000	7.947E-02	7.945E-02	7.816E-02	7.495E-02	6.016E-02	3.506E-02	8.858E-03	6.293E-05	7.300E-09
12.000	6.598E-02	6.597E-02	6.489E-02	6.222E-02	4.992E-02	2.907E-02	7.330E-03	5.174E-05	5.914E-09
14.000	5.643E-02	5.642E-02	5.550E-02	5.321E-02	4.268E-02	2.484E-02	6.258E-03	4.401E-05	4.996E-09
16.000	4.931E-02	4.930E-02	4.849E-02	4.649E-02	3.729E-02	2.170E-02	5.461E-03	3.833E-05	4.334E-09
18.000	4.378E-02	4.378E-02	4.306E-02	4.129E-02	3.311E-02	1.926E-02	4.846E-03	3.396E-05	3.830E-09
20.000	3.938E-02	3.937E-02	3.873E-02	3.713E-02	2.977E-02	1.732E-02	4.356E-03	3.050E-05	3.434E-09
25.000	3.147E-02	3.146E-02	3.094E-02	2.967E-02	2.379E-02	1.384E-02	3.478E-03	2.432E-05	2.731E-09

TABLE 2

$\frac{z}{z_D}$		$b(z, z_D)$										
		.01	.02	.1	.2	.5	1.0	2.0	5.0	10.0	100.0	∞
.000	.005	.010	.050	.101	.264	.535	.907	1.277	1.422	1.556	1.571	
.001	.005	.010	.050	.101	.263	.535	.907	1.277	1.422	1.556	1.571	
.002	.004	.010	.050	.101	.263	.535	.907	1.277	1.422	1.556	1.571	
.003	.004	.009	.050	.101	.262	.535	.907	1.277	1.422	1.556	1.571	
.004	.003	.009	.050	.100	.262	.535	.907	1.277	1.422	1.556	1.571	
.005	.003	.008	.050	.100	.262	.535	.907	1.277	1.422	1.556	1.571	
.006	.003	.008	.050	.100	.262	.534	.907	1.277	1.422	1.556	1.571	
.007	.002	.007	.049	.100	.262	.534	.907	1.277	1.421	1.556	1.570	
.008	.002	.007	.049	.100	.262	.534	.907	1.277	1.421	1.555	1.570	
.009	.002	.007	.049	.099	.262	.534	.906	1.277	1.421	1.555	1.570	
.010	.001	.006	.048	.099	.262	.534	.906	1.277	1.421	1.555	1.570	
.020	.000	.003	.044	.096	.260	.532	.905	1.275	1.419	1.553	1.568	
.030	.000	.001	.040	.092	.257	.530	.902	1.273	1.417	1.551	1.566	
.040	.000	.001	.035	.088	.253	.526	.899	1.269	1.413	1.547	1.562	
.050	.000	.000	.031	.083	.249	.523	.895	1.265	1.410	1.544	1.559	
.060	.000	.000	.026	.078	.245	.519	.891	1.261	1.405	1.539	1.554	
.070	.000	.000	.023	.074	.240	.514	.886	1.256	1.401	1.535	1.549	
.080	.000	.000	.020	.069	.236	.509	.881	1.251	1.395	1.529	1.544	
.090	.000	.000	.017	.064	.231	.505	.876	1.246	1.390	1.524	1.539	
.100	.000	.000	.014	.060	.226	.499	.870	1.240	1.384	1.518	1.533	
.200	.000	.000	.003	.028	.174	.440	.804	1.169	1.312	1.445	1.460	
.300	.000	.000	.000	.012	.128	.376	.728	1.085	1.227	1.360	1.375	
.400	.000	.000	.000	.005	.092	.316	.651	.999	1.138	1.270	1.285	
.500	.000	.000	.000	.002	.065	.263	.578	.913	1.050	1.182	1.196	
.600	.000	.000	.000	.001	.045	.217	.509	.832	.966	1.096	1.111	
.700	.000	.000	.000	.000	.031	.177	.447	.756	.887	1.016	1.031	
.800	.000	.000	.000	.000	.021	.145	.391	.685	.813	.941	.956	
.900	.000	.000	.000	.000	.015	.117	.341	.621	.746	.872	.887	
1.000	.000	.000	.000	.000	.010	.095	.297	.562	.684	.809	.823	
2.000	.000	.000	.000	.000	.000	.011	.073	.216	.306	.418	.433	
3.000	.000	.000	.000	.000	.000	.001	.019	.095	.162	.262	.276	
4.000	.000	.000	.000	.000	.000	.000	.005	.047	.097	.188	.202	
5.000	.000	.000	.000	.000	.000	.000	.002	.025	.063	.145	.160	
6.000	.000	.000	.000	.000	.000	.000	.001	.014	.043	.118	.132	
7.000	.000	.000	.000	.000	.000	.000	.000	.008	.031	.099	.113	
8.000	.000	.000	.000	.000	.000	.000	.000	.005	.022	.085	.099	
9.000	.000	.000	.000	.000	.000	.000	.000	.003	.016	.074	.088	
10.000	.000	.000	.000	.000	.000	.000	.000	.002	.012	.065	.079	

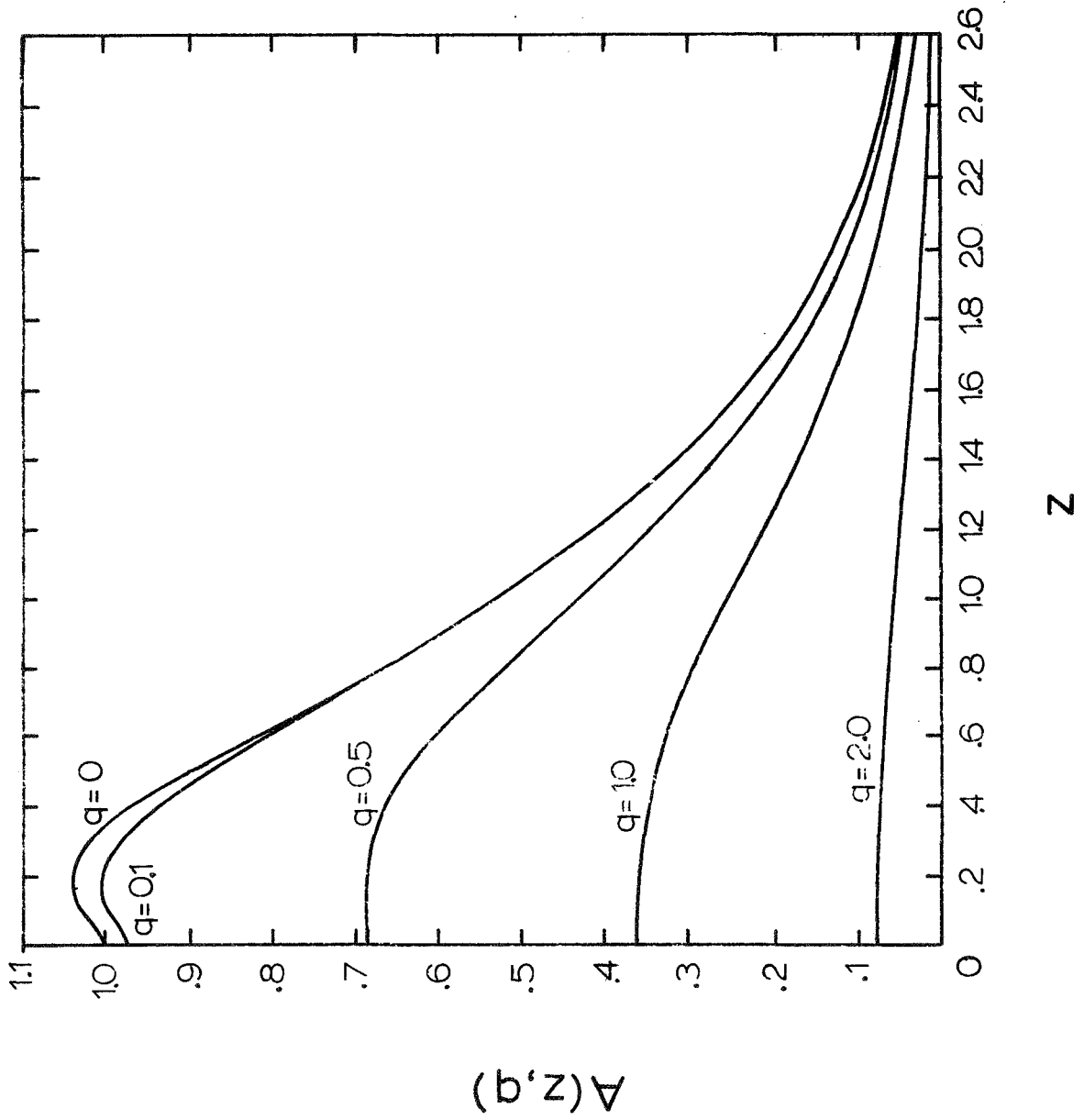


Figure 2

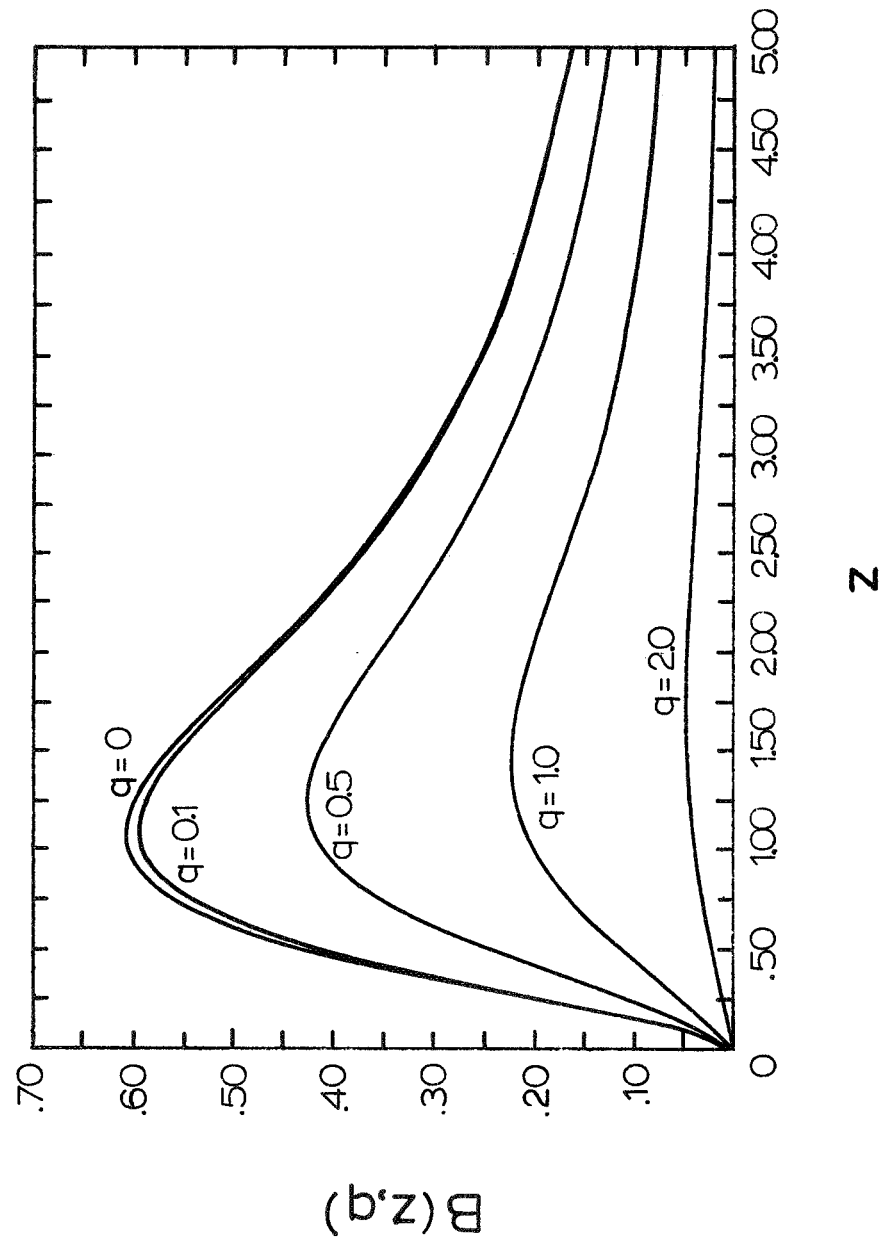


Figure 3

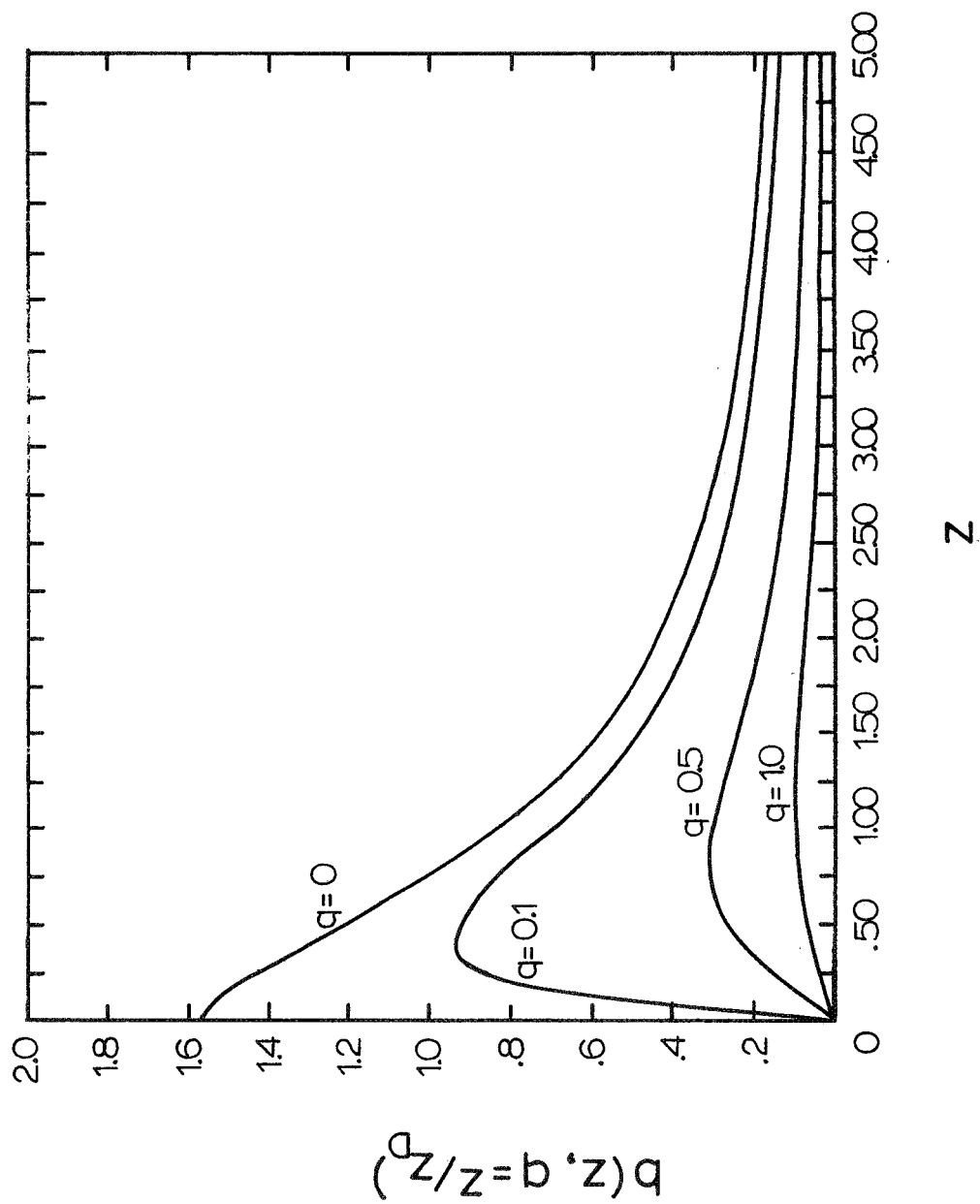
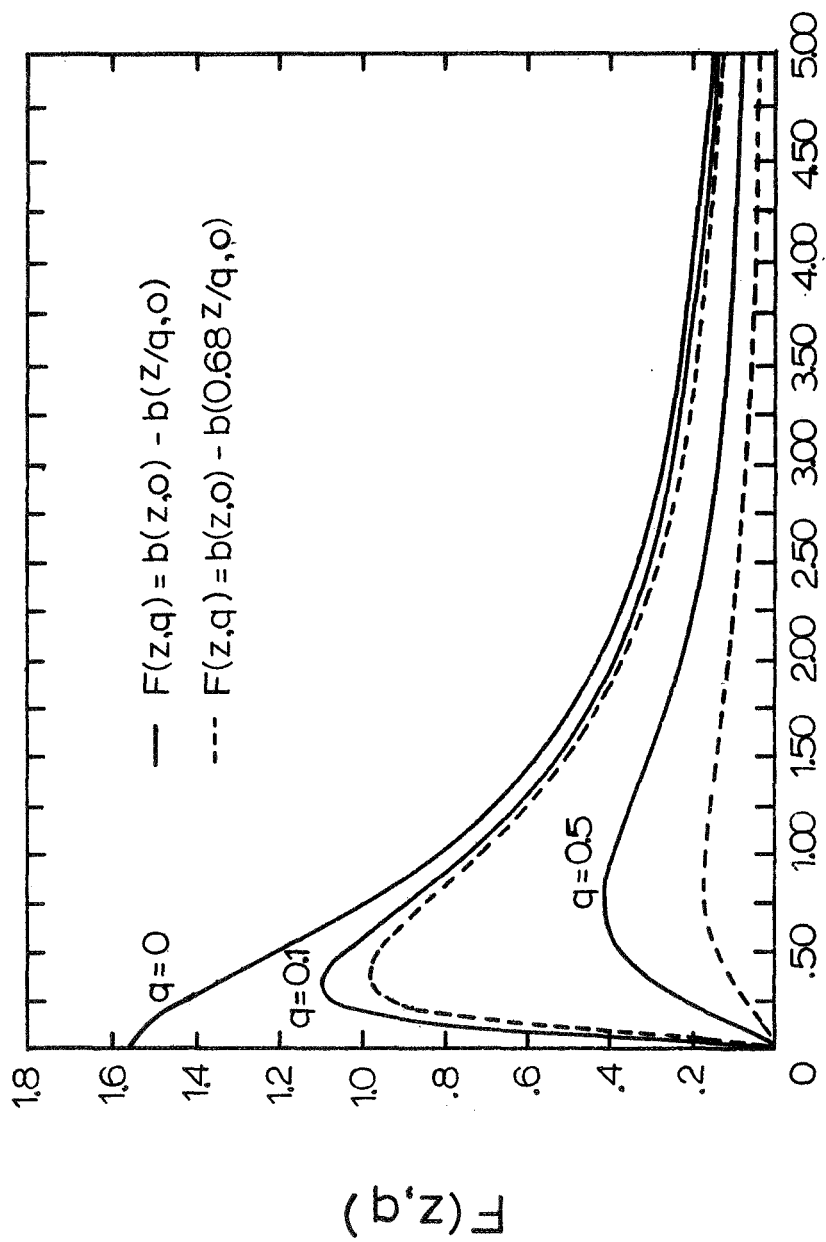


Figure 4



z

Figure 5

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APPENDIX

FORTTRAN Programs for $B(z,q)$ and $b(z,z_D)$

(Written by U. Palmer, Joint Institute for Laboratory Astrophysics)

$b(z,z_D)$

$b(z,z_D)$ is calculated by FUNCTION FOFZZD(Z,ZD)

A sample FORTRAN CALL: $B = \text{FOFZZD}(Z,ZD)$

FUNCTION FOFZZD requires the following seven routines and a data deck

marked $b(z,z_D)$

1. FUNCTION B2(Z)
2. FUNCTION FACT(N)
3. SUBROUTINE KI1(X,CAY)
4. SUBROUTINE INTERP(NX,NY,X,Y,Z,R,S,T)
5. SUBROUTINE LAGRANG(NPTS,X,Y,NP,LAP,ISTART,IEND,LEND,R,V)
6. SUBROUTINE BESSK(X,CKE,EI)
7. SUBROUTINE BESSI(X,EI)
8. data deck $b(z,z_D)$

$B(z,q)$

$B(z,q)$ is calculated by FUNCTION FOFZQ(ZZ,QQ)

A sample FORTRAN CALL: $B = \text{FOFZQ}(Z,Q)$

The following routines are needed by FUNCTION FOFZQ(ZZ,QQ)

- A. SUBROUTINE INTPB
- B. FUNCTION BQASYM(Z,Q)
- C. ROUTINES numbered 2-7 on the list for $b(z,z_D)$
- D. data deck marked $B(Z,Q)$

Use of FUNCTIONS FOFZQ(ZZ,QQ) and FOFZZD(Z,ZD)

$b(z, z_D)$ and $B(z, q)$ are calculated by interpolating in tables $B(Z, ZD)$ and $B(Z, Q)$ respectively. Accuracy within the $B(z, q)$ table exceeds 2%. When $b(z, z_D)$ exceeds 0.01 the accuracy is also better than 2%, between 0.01 and 0.001 the first non-zero digit is definitely significant and, when less than 0.001, $b(z, z_D) = 0$ will be returned. The tables are provided by the data decks marked $b(z, z_D)$ and $B(z, q)$.

The first call to either routine will cause the reading of its own data deck. When inserting the routines into an already existing program, care must be taken in arranging the data. Therefore, it would be best to make dummy calls to FOFZZD and FOFZQ in the beginning of the main program and at the same time placing the data decks at the start of the program's whole data set.

For example:

PROGRAM: PROGRAM MAIN

DUMMY = FOFZQ(2.0,2.0) causes reading of table $B(Z, Q)$ and

stores $B(2.0, 2.0)$ into DUMMY

DUMMI = FOFZZD(2.0,2.0) causes reading of table $b(z, z_D)$ and

stores $b(2.0, 2.0)$ into DUMMI

rest of program

END

DATA: Table $B(Z, Q)$

Table $b(z, z_D)$

rest of data for Program Main

PROGRAM TESTBS (INPUT,OUTPUT)	001
DIMENSION ZZZ(25),QQQ(25)	002
DUMMY = FOFZQ(2.0,2.0)	003
DUMMI = FOFZZD(2.0,2.0)	004
PRINT 600	005
10 CONTINUE	006
READ 500,NZZZ,NQQQ	007
IF(NZZZ.LT.0) CALL EXIT	008
READ 501,(ZZZ(I),I=1,NZZZ)	009
READ 501,(QQQ(I),I=1,NQQQ)	010
DO 400 J = 1,NQQQ	011
PRINT 670	012
670 FORMAT(1H0)	013
Q = QQQ(J)	014
DO 400 I = 1,NZZZ	015
Z = ZZZ(I)	016
BZQ = FOFZQ(Z,Q)	017
BZZD = FOFZZD(Z,Q)	018
PRINT 601,Z,Q,BZQ,BZZD	019
400 CONTINUE	020
500 FORMAT(20I4)	021
501 FORMAT(5E15.0)	022
600 FORMAT(1H1,18X,*Z*,13X,*Q OR ZD*,13X,*B (Z,Q)*,12X,*B (Z,ZD)*,//)	023
601 FORMAT(4F20.8)	024
END	025

	FUNCTION FOFZZD(Z,ZD)	360
	COMMON/SETBZZD/B(38,21),ZE(38),ZEDE(21),ZLIM(14),Y(5),NZ,NZD,NZLIM	361
	DIMENSION CK(3),CEI(3)	362
	DATA(LSWITCH = 1)	363
	GO TO (1,2),LSWITCH	364
	1 LSWITCH = 2	365
C		366
C	READ B(Z,ZD) DATA DECK	367
C		368
	READ 500,NZ,NZD,NZLIM	369
	READ 501,(ZE(I),I=1,NZ)	370
	DO 110 J = 1,NZD	371
	READ 501,ZEDE(J)	372
	READ 501,(B(I,J),I=1,NZ)	373
110	CONTINUE	374
	PRINT 600,(ZEDE(IU),IU = 1,10)	375
	PRINT 601,(ZE(IU),(B(IU,LU),LU=1,10),IU = 1,NZ)	376
	PRINT 603,(ZEDE(IU),IU = 11,NZD)	377
	PRINT 604,(ZE(IU),(B(IU,LU),LU=11,NZD),IU = 1,NZ)	378
	READ 501,(ZLIM(I), I= 1,NZLIM)	379
	DO 120 I = 1,5	380
	Y(I) = ALOG10(ZEDE(I+16))	381
120	CONTINUE	382
C		383
C	CALCULATE B(Z,ZD)	384
C		385
	2 IF(ZD.GE.0.001) GO TO 10	386
	5 FOFZZD = 0.0	387
	RETURN	388
10	IF((ZD.LT.2.0).AND.(Z.GT.10.0)) GO TO 5	389
	DO 20 J = 2,NZLIM	390
	IF((ZD.LE.ZEDE(J)).AND.(Z.GT.ZLIM(J)))5,20	391
20	CONTINUE	392
	IF((ZD.LT..1) .OR.(Z.GT.10.0)) GO TO 30	393
	IF(ZD.GT.20000.0) GO TO 40	394
	IF((ZD.GE.10.0).AND.(ZD.LE.2000.0)) GO TO 50	395
		396
C		397
C	LAG. INTERP	398
C		399
	CALL INTERP(NZD,NZ,ZEDE,ZE,B,ZD,Z,TEMP,4)	400
	FOFZZD = TEMP	401
	GO TO 200	402
C		403
C	B(Z,ZD) ASYM	404
C		405
30	ZZD = Z/ZD	406
	TZZD = 2.0*ZZD	407
	CALL BESSK(TZZD,CK,CEI)	408
	FK0 = CK(1)	409
	FK1 = CK(2)	410
	IF(ZD.LT.0.1) GO TO 60	411
	CALL K11(TZZD,FK11)	412
	TZZDSQ = TZZD * ZZD	413
	FOFZZD = (1./(2.*Z))*(FK11*(1.+TZZDSQ)-TZZDSQ*FK1+TZZD*FK0)	414
	GO TO 200	415
C		416
C	B2(Z)	417
C		418
40	FOFZZD = B2(Z)	419
	GO TO 200	

C		420
C	LOG INTERP	421
C		422
	50 CALL INTERP(5,NZ,Y,ZE,B(1,17),ALOG10(ZD),Z,TEMP,2)	423
	FOFZZD = TEMP	424
	GO TO 200	425
	60 FOFZZD = Z * FK1	426
	200 IF(FOFZZD.LT.0.001) FOFZZD = 0.0	427
	RETURN	428
	500 FORMAT(20I4)	429
	501 FORMAT(10F8.4)	430
	600 FORMAT(1H1,*B(Z,ZD)*,/,*, ZD*,3X,10F10.3,/,*, Z*,/)	431
	601 FORMAT(F8.4,10F10.5)	432
	602 FORMAT(1H1,*B(Z,ZD)*,/,*, ZD*,3X,11F10.3,/,*, Z*,/)	433
	604 FORMAT(F8.4,11F10.5)	434
	END	435

	FUNCTION B2(Z)	436
	DIMENSION C(3),EI(3)	437
	PI = 3.141592654	438
	CALL BESSK (Z,C,EI)	439
	B2 = 0.5 * PI - PI * Z * C(1) * FI(2)	440
	RETURN	441
	END	442

	FUNCTION FACT (N)	176
	DOUBLE F	177
	F = 1.0	178
	IF(N .GE. 0) GO TO 10	179
	PRINT 600	180
	600 FORMAT(1H0,*NEGATIVE FACTORIAL*)	181
	CALL EXIT	182
	10 FACT = 1.0	183
	IF(N.GT. 1).GOTO 20	184
	RETURN	185
	20 DO 30 I = 1,N	186
	F = F * I	187
	30 CONTINUE	188
	FACT = F	189
	RETURN	190
	END	191

```

SUBROUTINE KI1(X,CAY)
DIMENSION EK(7)
DATA(PI=3.141592654),(EK=1.25331414,0.11190289,0.02576646,
1      0.00933994,0.00417454,0.00163271,0.00033934)
DATA(EULER= 0.5772156649)
PI2 = PI/2.0
IF(X.NE.0.0) GO TO 10
CAY = PI2
RETURN
10 IF(X.GT.7.0) GO TO 200
XT = X/2.0
EPS = 1.0E-9
COEF = -(EULER+ALOG(XT))*X
SUM = 0.0      $      SUMA=0.0
SUMB = 0.0     $      SUMC = 0.0
KB = 0
DO 100 K = KB,100
TM = 2*K+1
TK = FACT(K)**2
TN = XT**(2*K)
TA = TN/(TK*TM)
TB = TN / (TK*TM**2)
SUM = SUM + 1.0 / (K+1.0)
TC = (XT**(2*(K+1)))/(FACT(K+1)**2*(2*(K+1)+1))*SUM
SUMA = SUMA + TA
SUMB = SUMB + TB
SUMC = SUMC + TC
IF(ABS (TA) .GT. EPS *ABS (SUMA)) GO TO 100
IF(ABS (TB) .GT. EPS *ABS (SUMB)) GO TO 100
IF(ABS (TC) .GT. EPS *ABS (SUMC)) GO TO 100
GO TO 150
100 CONTINUE
C PRINT 600,TA,TB,TC,SUM,SUMA,SUMB,SUMC,K
600 FORMAT(40X,7E13.5,I5)
CALL EXIT
150 CAY = PI2 - COEF*SUMA - X*SUMB -X *SUMC
C PRINT 600,TA,TB,TC,SUM,SUMA,SUMB,SUMC,K
RETURN
200 X7 = X/7.0      $      SUMD = 0.0
DO 250 M=1,7
SUMD = SUMD +      (-1.0)**(M-1) * EK(M) / X7**(M-1)
250 CONTINUE
CAY = SUMD/(SQRT(X) * EXP(X))
RETURN
END

```

SUBROUTINE INTERP(NX,NY,X,Y,Z,R,S,T,NP)	275
DIMENSION X(NX),Y(NY),Z(NY,NX)	276
DIMENSION DIN(20),STORE(20)	277
NPTS = 4	278
DO 10 N = 2,NX	279
IF(R.GT.X(N)) 10,20	280
10 CONTINUE	281
15 PRINT 600,R,S,X(NX),Y(NY)	282
CALL EXIT	283
600 FORMAT(*0R,S,X(NX),Y(NY)*,4E20.9,//)	284
20 NP = N-1	285
DO 30 N = 2,NY	286
IF(S.GT.Y(N)) 30,40	287
30 CONTINUE	288
GO TO 15	289
40 NS = N - 1	290
IF(NS.EQ.1) NS = NS + 1	291
IF(NR.EQ.1) NR = NR + 1	292
IF(NS.EQ.(NY-1)) NS = NS - 1	293
IF(NR.EQ.(NX-1)) NR = NR - 1	294
DO 100 I = 1,4	295
II = NR-2+I	296
DO 50 J = 1,4	297
JJ = NS-2+J	298
DIN(J) = Z(JJ,II)	299
50 CONTINUE	300
CALL LAGRANG(4,Y (NS-1),DIN,NPTS,NPTS-1,1,1,LEND,S ,STORE(I))	301
100 CONTINUE	302
CALL LAGRANG(4,X (NR-1),STORE,NPTS,NPTS-1,1,1,LEND,R,T)	303
RETURN	304
END	305

SUBROUTINE LAGRANG (NPTS,X,Y,NP,LAP,ISTART,IEND,LEND,R,V)	306
DIMENSION X(NPTS),Y(NPTS),R(IEND),V(IEND),DN(15),DD(15)	307
DO 100 I = 1,15	308
DN(I) = 1.	309
100 DD(I) = 1.	310
LT = NP/2 - 1	311
NPMLAP = NP - LAP	312
NI = 1	313
NE = NP	314
NTEMP = 0	315
IR = ISTART	316
102 IF(R(IR) - X(NE-LT)) 102,102,101	317
101 IF((NE.EQ.NPTS).AND.(R(IR).LE.X(NE)))GO TO 102	318
NI = NI + NPMLAP	319
NE = NE + NPMLAP	320
NTEMP = NI - 1	321
IF(NE - NPTS)103,103,104	322
104 LEND = IR - 1	323
RETURN	324
102 DO 110 K = 1,NP	325
KK = K + NTEMP	326
DO 110 I = 1,NP	327
II = I + NTEMP	328
IF(K-I)108,110,108	329
108 DD(K) = DD(K) * (X(KK) - X(II))	330
110 CONTINUE	331
112 V(IR) = 0.0	332
DO 120 IT = NI,NE	333
IF(R(IR) - X(IT))120,111,120	334
111 V(IR) = Y(IT)	335
GO TO 140	336
120 CONTINUE	337
DO 130 K = 1,NP	338
KK = K + NTEMP	339
DO 140 I = 1,NP	340
II = I + NTEMP	341
IF(K-I)141,140,141	342
141 DN(K) = DN(K) * (R(IR) - X(II))	343
140 CONTINUE	344
V(IR) = V(IR) + (DN(K) * Y(KK) / DD(K))	345
130 CONTINUE	346
149 IF(IR - IEND)150,151,151	347
150 IR = IR + 1	348
DO 170 MZ = 1,NP	349
170 DN(MZ) = 1.0	350
IF(R(IR) - X(NE - LT))112,112,161	351
161 IF(NE .LT. NPTS) GO TO 162	352
IF(R(IR) .LE. X(NPTS)) GO TO 112	353
162 DO 180 MZ = 1,NP	354
180 DD(MZ) = 1.0	355
GO TO 101	356
151 LEND = IEND	357
RETURN	358
END	359

	SUBROUTINE BESSK (X,CKE,EI)	192
	DIMENSION FIRST(4),EI(3),COEF(4),CKE(3),A(10,4)	193
	DATA (A = 0.42278420, .23069756, .03488590,	194
1	.00262698, .00010750, .00000740, 3(0.0), 6.0,	195
2	.15443144, -.67278579, -.18156897,	196
3	-.01919407, -.00110404, -.00004686, 3(0.0), 6.0,	197
4	-.07832358, .02189568, -.01062446,	198
5	.00587872, -.00251540, .00053208, 3(0.0), 6.0,	199
6	.23498619, -.03655620, .01504268,	200
7	-.00780353, .00325614, -.00068245, 3(0.0), 6.0)	201
	CALL BESSI (X,EI)	202
	IF(X .LT. 2.0) 10,20	203
10	T = X / 2.0	204
	XP = ALOG(T)	205
	FIRST(1) = -XP * EI(1) - 0.57721566	206
	FIRST(2) = X * XP * EI(2) + 1.0	207
	FACTOR = T * T	208
	COEF(1) = 1.0	209
	COEF(2) = 1.0 / X	210
	JJ = 1	211
	GO TO 50	212
20	T = 2.0 / X	213
	FIRST(3) = FIRST(4) = 1.25331414	214
	JJ = 3	215
	COEF(3) = COEF(4) = 1.0 / (SQRT (X) * EXP (X))	216
	FACTOR = T	217
50	JEND = JJ + 1	218
	I = 0	219
	DO 200 J = JJ,JEND	220
	I = I + 1	221
	PROD = 1.0	222
	SUM = 0.0	223
	KEND = A(10,J) + 0.000001	224
	DO 100 K = 1,KEND	225
	PROD = PROD * FACTOR	226
	SUM = SUM + PROD * A(K,J)	227
100	CONTINUE	228
	CKE(1) = COEF(J) * (FIRST(J) + SUM)	229
200	CONTINUE	230
	CKE(3) = (2.0/X) * CKE(2) + CKE(1)	231
	RETURN	232
	END	233

SUBROUTINE BESSI (X,EI)		224
DIMENSION A(10,4),FIRST(4),COEF(4),EI(3)		225
DATA(FIRST = 1.0,0.5,2(0.39894228)),		226
1 (A= 3.5156229, 3.0899424, 1.2067492,		227
2 .2659732, .0360768, .0045813, 3(0.0), 6.0,		228
3 .87890594, .51498869, .15084934,		229
4 .02658733, .00301532, .00032411, 3(0.0), 6.0,		240
5 .01328592, .00225319,-.00157565,		241
6 .00916281, -.02057706, .02635537,		242
7 -.01647633, .00392377, 0.0 , 8.0,		243
8 -.03988024, -.00362018, .00163801,		244
9 -.01031555, .02282967,-.02895312,		245
1 .01787654, -.00420059, 0.0 , 8.0)		246
		247
T = X / 3.75		248
COEF(1) = 1.0		249
COEF(2) = X		250
COEF(3) = COEF(4) = EXP (X) / SQRT (X)		251
IF(X .LT. 3.75) 10,20		252
10 FACTOR = T * T		253
JJ = 1		254
GO TO 50		255
20 FACTOR = 1.0 / T		256
JJ = 3		257
50 JEND = JJ + 1		258
I = 0		259
DO 200 J = JJ,JEND		260
I = I + 1		261
PROD = 1.0		262
SUM = 0.0		263
KEND = A(10,J) + .000001		264
DO 100 K = 1,KEND		265
PROD = PROD * FACTOR		266
SUM = SUM + PROD * A(K,J)		267
100 CONTINUE		268
EI(1) = COEF(J) * (FIRST(J) + SUM)		269
200 CONTINUE		270
		271
EI(3) = (-2.0/X) * EI(2) + EI(1)		272
RETURN		273
END		274

38	21	14								
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
.01	.02	.03	.04	.05	.06	.07	.08	.09	.1	.2
.3	.4	.5	.6	.7	.8	.9	10.			
.0010	.0005	.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
.0050	.0025	.0022	.0017	.0013	.0010	.0007	.0005	.0004	.0003	.0002
.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
.01	.0050	.0048	.0044	.0039	.0034	.0030	.0026	.0022	.0019	.0016
.0014	.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
.02	.0100	.0099	.0096	.0092	.0087	.0083	.0078	.0074	.0069	.0065
.0060	.0028	.0012	.0005	.0002	.0001	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
.0500	.0250	.0248	.0246	.0243	.0240	.0236	.0232	.0228	.0224	.0224
.0219	.0173	.0131	.0097	.0071	.0051	.0036	.0026	.0018	.0013	.0013
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
.1	.0502	.0505	.0504	.0503	.0501	.0499	.0496	.0493	.0490	.0487
.0483	.0442	.0396	.0350	.0306	.0265	.0229	.0197	.0169	.0144	.0144
.0025	.0004	.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
.1500	.0755	.0764	.0763	.0762	.0760	.0759	.0757	.0754	.0752	.0749
.0746	.0711	.0668	.0622	.0574	.0528	.0483	.0441	.0401	.0364	.0364
.0121	.0037	.0011	.0003	.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
.2	.1012	.1008	.1007	.1006	.1005	.1003	.1002	.1000	.0998	.0995
.0993	.0962	.0922	.0878	.0831	.0783	.0736	.0689	.0643	.0599	.0599
.0276	.0118	.0048	.0019	.0008	.0003	.0001	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
.3000	.1538	.1531	.1531	.15						

1.									
.5354	.5347	.5346	.5346	.5345	.5345	.5344	.5343	.5342	.5340
.5339	.5321	.5296	.5265	.5228	.5187	.5143	.5095	.5045	.4992
.4396	.3762	.3164	.2629	.2167	.1774	.1446	.1174	.0950	.0105
.0011	.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000		
1.5000									
.7520	.7516	.7516	.7515	.7515	.7514	.7513	.7512	.7511	.7510
.7509	.7491	.7466	.7435	.7399	.7357	.7312	.7263	.7212	.7157
.6518	.5804	.5096	.4430	.3826	.3287	.2813	.2400	.2043	.0388
.0074	.0015	.0003	.0001	0.0000	0.0000	0.0000	0.0000		
2.									
.9072	.9070	.9070	.9070	.9069	.9068	.9067	.9067	.9065	.9064
.9063	.9046	.9020	.8989	.8952	.8910	.8864	.8814	.8761	.8705
.8040	.7282	.6513	.5777	.5093	.4470	.3911	.3413	.2974	.0730
.0187	.0052	.0015	.0005	.0002	.0001	0.0000	0.0000		
3.0000									
1.0990	1.0992	1.0992	1.0992	1.0991	1.0990	1.0990	1.0989	1.0988	1.0986
1.0985	1.0967	1.0942	1.0910	1.0873	1.0830	1.0783	1.0732	1.0678	1.0620
.9928	.9125	.8298	.7492	.6731	.6026	.5381	.4796	.4271	.1346
.0463	.0177	.0073	.0032	.0014	.0007	.0003	.0001		
5.									
1.2773	1.2775	1.2775	1.2775	1.2774	1.2773	1.2772	1.2771	1.2770	1.2769
1.2768	1.2750	1.2725	1.2692	1.2654	1.2611	1.2563	1.2512	1.2457	1.2398
1.1687	1.0854	.9988	.9135	.8320	.7558	.6854	.6209	.5622	.2163
.0947	.0468	.0251	.0142	.0083	.0049	.0030	.0018		
10.									
1.4216	1.4218	1.4218	1.4217	1.4217	1.4216	1.4215	1.4214	1.4213	1.4212
1.4211	1.4193	1.4167	1.4135	1.4096	1.4053	1.4005	1.3953	1.3897	1.3838
1.3117	1.2269	1.1382	1.0504	.9662	.8870	.8134	.7456	.6836	.3064
.1615	.0971	.0632	.0433	.0306	.0221	.0162	.0121		
100.									
1.5558	1.5559	1.5558	1.5558	1.5557	1.5556	1.5556	1.5555	1.5554	1.5552
1.5551	1.5533	1.5507	1.5475	1.5436	1.5393	1.5345	1.5292	1.5236	1.5177
1.4453	1.3598	1.2703	1.1816	1.0964	1.0160	.9411	.8720	.8087	.4180
.2616	.1875	.1454	.1181	.0990	.0849	.0739	.0652		
1000.									
1.5693	1.5692	1.5692	1.5692	1.5691	1.5690	1.5690	1.5689	1.5688	1.5686
1.5685	1.5667	1.5641	1.5609	1.5570	1.5527	1.5478	1.5426	1.5370	1.5311
1.4587	1.3732	1.2837	1.1950	1.1097	1.0293	.9544	.8853	.8219	.4312
.2746	.2003	.1581	.1307	.1114	.0971	.0861	.0772		
10000.									
1.5707	1.5701	1.5701	1.5700	1.5700	1.5699	1.5698	1.5697	1.5696	1.5695
1.5694	1.5676	1.5650	1.5617	1.5579	1.5535	1.5487	1.5435	1.5379	1.5319
1.4595	1.3741	1.2845	1.1958	1.1106	1.0301	.9553	.8862	.8228	.4320
.2754	.2012	.1589	.1315	.1123	.0980	.0869	.0781		
20000.									
1.5707	1.5701	1.5701	1.5700	1.5700	1.5699	1.5698	1.5697	1.5696	1.5695
1.5694	1.5676	1.5650	1.5617	1.5579	1.5535	1.5487	1.5435	1.5379	1.5319
1.4595	1.3741	1.2846	1.1958	1.1106	1.0301	.9553	.8862	.8228	.4320
.2754	.2012	.1589	.1315	.1123	.0980	.0869	.0781		
.001	.01	.02	.06	.1	.4	.6	.8	1.	2.
3.	4.	6.	8.						

FUNCTION FOFZQ(ZZ,QQ)	026
COMMON /DAT/ Z(45),Q(17),B(45,17),NZ,NQ,NPTS	027
COMMON/ORIG/BB(45,17),PI	028
COMMON/NSM/ BNSM(45,17)	029
DIMENSION EI(3),CKE(3)	030
DATA(LSWITCH = 1)	031
DATA(PI = 3.141592654)	032
GO TO (100,200),LSWITCH	033
100 LSWITCH = 2	034
C READ DATA DECK B(Z,Q) AND GENERATE SMOOTHED TABLES FOR B(Z,Q)	035
C	036
C CALL INTPB	037
C	038
C CALCULATE B(Z,Q)	039
C	040
200 IF(QQ.GT.0.0) GO TO 201	041
CALL BESSK(ZZ,CKE,EI)	042
FOFZQ = PI * ZZ**2 * (CKE(1)*EI(1) - CKE(2) * EI(2))	043
RETURN	044
201 IF(QQ.LT.10.0) GO TO 10	045
5 FOFZQ = 0.0	046
RETURN	047
10 TEMPB = BOASYM(ZZ,QQ)	048
IF(ZZ.LT.Z(1)) GO TO 5	049
IF(ZZ.LE.0.05) GO TO 30	050
IF(ZZ.LE.25.0) GO TO 40	051
FOFZQ = TEMPB	052
RETURN	053
20 CALL INTERP(NQ,NZ,Q,Z,BNSM,QQ,ZZ,TEMP,NPTS)	054
TZ = ZZ**2	055
TQ = 2.0 * QQ	056
RTZTQ = SQRT(TZ+TQ**2)	057
CALL BESSK(RTZTQ,CKE,EI)	058
DENUM = PI*ZZ*SQRT(TZ+(TQ/PI)**2) * CKE(1)	059
FOFZQ = TEMP * DENUM	060
RETURN	061
40 CALL INTERP(NQ,NZ,Q,Z,B ,QQ,ZZ,TEMP,NPTS)	062
CALL LAGRANG (NZ,Z,BB(1,1),4,3,1,1,LEND,ZZ,BBB)	063
TB = TEMP * BBB * (4.0*ZZ/PI) * TEMPB	064
FOFZQ = TB	065
RETURN	066
END	067

	SUBROUTINE INTPB	078
	COMMON /DAT/ Z(45),Q(17),B(45,17),NZ,NQ,NPTS	079
	COMMON/ORIG/ P(45,17),PI	080
	COMMON/NSM/ BNSM(45,17)	081
	DIMENSION C(3),EI(3)	082
	NZ = 45	083
	NQ = 17	084
	PI = 3.141592654	085
	NPTS = 4	086
C		087
C	READ DATA DECK FOR B(Z,Q)	088
C		089
	5 READ 501,(Z(I),I=1,NZ)	090
	DO 10 J = 1,NQ	091
	READ 502,Q(J)	092
	READ 502,(P(I,J),I=1,NZ)	093
10	CONTINUE	094
C		095
C	PRINT TABLE B(Z,Q)	096
C		097
	PRINT 612,(Q(I),I=1,9)	098
	PRINT 613	099
	PRINT 611,(Z(I),(P(I,J),J=1,9),I=1,NZ)	100
	PRINT 612,(Q(I),I=10,NQ)	101
	PRINT 613	102
	DO 1509 I = 1,NZ	103
	PRINT 611,(Z(I),(P(I,J),J=10,NQ))	104
1509	CONTINUE	105
	DO 15 I = 1,NZ	106
C		107
C	SMOOTH TABLE B(Z,Q) FOR Z .LE. 0.05	108
C		109
	B(I,1) = 1.0	110
	TEMP = 4.0*Z(I)/PI	111
	DO 13 IY = 1,NQ	112
	TBNSM = SQRT(Z(I)**2+(2.0*Q(IY))**2)	113
	CALL BESSK(TBNSM,C,EI)	114
	DENEW = PI*Z(I) * SQRT(Z(I)**2+(2.0*Q(IY)/PI)**2)*C(1)	115
	BNSM(I,IY) = P(I,IY)/DENEW	116
13	CONTINUE	117
C		118
C	SMOOTH TABLE B(Z,Q) FOR Z .GT. 0.05 AND Z .LE. 25.0	119
C		120
	DO 15 J = 2,NQ	121
	B(I,J) = (P(I,J)/P(I,1)) / (TEMP*BQASYM(Z(I),Q(J)))	122
15	CONTINUE	123
501	FORMAT(10F8.0)	124
502	FORMAT(6E12.4)	125
611	FORMAT(F10.3,9E14.4)	126
612	FORMAT(1H1,*B(Z,Q)*,/,7X,*Q*,2X,9F14.3,/,)	127
613	FORMAT(1H,* Z*,/,)	128
	RETURN	129
	END	130

FUNCTION BQASYM(Z,Q)	060
DIMENSION CK(3),CEI(3)	070
TWOQ = 2.0 * Q	071
CALL BESSK(TWOQ,CK,CEI)	072
CALL KI1(TWOQ,CAY)	073
QSQ = Q**2	074
BQASYM = (1.0/Z)*((0.5-QSQ)*CAY+Q*CK(1) + 2.0*QSQ * CK(2))	075
RETURN	076
END	077

0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009	0.010
0.020	0.030	0.040	0.050	0.060	0.070	0.080	0.090	0.100	0.200
0.300	0.400	0.500	0.600	0.700	0.800	0.900	1.000	1.200	1.400
1.600	1.800	2.000	3.000	4.000	5.000	6.000	8.000	10.000	12.000
14.000	16.000	18.000	20.000	25.000					
1.0000E-08									
2.0495E-05	7.3269E-05	1.5339E-04	2.5824E-04	3.8597E-04	5.3519E-04				
7.0472E-04	8.9362E-04	1.1010E-03	1.3262E-03	4.4350E-03	8.8363E-03				
1.4272E-02	2.0564E-02	2.7577E-02	3.5205E-02	4.3356E-02	5.1957E-02				
6.0942E-02	1.6214E-01	2.6576E-01	3.5884E-01	4.3662E-01	4.9806E-01				
5.4397E-01	5.7594E-01	5.9594E-01	6.0592E-01	6.0312E-01	5.8005E-01				
5.4588E-01	5.0684E-01	4.6690E-01	2.0545E-01	2.1582E-01	1.6625E-01				
1.3578E-01	1.0006E-01	7.9469E-02	6.5978E-02	5.6429E-02	4.9306E-02				
4.3785E-02	3.9379E-02	3.1470E-02							
5.0000E-03									
4.8939E-05	1.0761E-04	1.8318E-04	2.7951E-04	3.9791E-04	5.3832E-04				
7.0001E-04	8.8208E-04	1.0836E-03	1.3037E-03	4.3862E-03	8.7779E-03				
1.4209E-02	2.0498E-02	2.7510E-02	3.5136E-02	4.3286E-02	5.1887E-02				
6.0871E-02	1.6207E-01	2.6569E-01	3.5878E-01	4.3656E-01	4.9801E-01				
5.4391E-01	5.7590E-01	5.9589E-01	6.0588E-01	6.0309E-01	5.8002E-01				
5.4586E-01	5.0682E-01	4.6688E-01	3.0544E-01	2.1581E-01	1.6624E-01				
1.3578E-01	1.0005E-01	7.9466E-02	6.5976E-02	5.6427E-02	4.9304E-02				
4.3784E-02	3.9379E-02	3.1471E-02							
1.0000E-02									
8.1654E-05	1.6695E-04	2.6092E-04	3.6659E-04	4.8655E-04	6.2265E-04				
7.7606E-04	9.4739E-04	1.1368E-03	1.3444E-03	4.3253E-03	8.6646E-03				
1.4067E-02	2.0338E-02	2.7338E-02	3.4956E-02	4.3101E-02	5.1697E-02				
6.0678E-02	1.6187E-01	2.6550E-01	3.5859E-01	4.3639E-01	4.9785E-01				
5.4377E-01	5.7576E-01	5.9577E-01	6.0576E-01	6.0298E-01	5.7993E-01				
5.4578E-01	5.0675E-01	4.6682E-01	3.0540E-01	2.1578E-01	1.6622E-01				
1.3576E-01	1.0004E-01	7.9454E-02	6.5965E-02	5.6418E-02	4.9296E-02				
4.3776E-02	3.9372E-02	3.1463E-02							
5.0000E-02									
2.4279E-04	4.8608E-04	7.3038E-04	9.7618E-04	1.2240E-03	1.4742E-03				
1.7275E-03	1.9841E-03	2.2446E-03	2.5093E-03	5.4762E-03	9.2111E-03				
1.3840E-02	1.9355E-02	2.5681E-02	3.2723E-02	4.0382E-02	4.8571E-02				
5.7211E-02	1.5688E-01	2.6024E-01	3.5343E-01	4.3144E-01	4.9318E-01				
5.3939E-01	5.7167E-01	5.9195E-01	6.0221E-01	5.9989E-01	5.7723E-01				
5.4340E-01	5.0464E-01	4.6494E-01	3.0420E-01	2.1490E-01	1.6553E-01				
1.3519E-01	9.9613E-02	7.9116E-02	6.5684E-02	5.6177E-02	4.9086E-02				

4.4588E-04	8.9169E-04	1.3377E-03	1.7838E-03	2.2301E-03	2.6766E-03
3.1235E-03	3.5707E-03	4.0183E-03	4.4663E-03	8.9816E-03	1.3593E-02
1.8345E-02	2.3275E-02	2.8419E-02	3.3802E-02	3.9446E-02	4.5363E-02
5.1561E-02	1.2737E-01	2.1635E-01	3.0292E-01	3.7876E-01	4.4073E-01
4.8848E-01	5.2298E-01	5.4580E-01	5.5870E-01	5.6152E-01	5.4348E-01
5.1363E-01	4.7825E-01	4.4138E-01	2.8933E-01	2.0413E-01	1.5705E-01
1.2817E-01	9.4392E-02	7.4952E-02	6.2221E-02	5.3212E-02	4.6494E-02
4.1287E-02	3.7132E-02	2.9672E-02			
3.5000E-01					
4.6237E-04	9.2475E-04	1.3872E-03	1.8496E-03	2.3121E-03	2.7747E-03
3.2374E-03	3.7001E-03	4.1630E-03	4.6260E-03	9.2662E-03	1.3935E-02
1.8645E-02	2.3409E-02	2.8241E-02	3.3150E-02	3.8147E-02	4.3240E-02
4.8438E-02	1.0680E-01	1.7469E-01	2.4499E-01	3.1070E-01	3.6751E-01
4.1354E-01	4.4859E-01	4.7336E-01	4.8904E-01	4.9851E-01	4.8728E-01
4.6371E-01	4.3384E-01	4.0170E-01	2.6451E-01	1.8626E-01	1.4304E-01
1.1662E-01	8.5800E-02	6.8105E-02	5.6526E-02	4.8336E-02	4.2230E-02
3.7499E-02	3.3724E-02	2.6949E-02			
5.0000E-01					
4.2102E-04	8.4206E-04	1.2631E-03	1.6842E-03	2.1052E-03	2.5263E-03
2.9475E-03	3.3686E-03	3.7899E-03	4.2111E-03	8.4275E-03	1.2654E-02
1.6897E-02	2.1160E-02	2.5449E-02	2.9767E-02	3.4119E-02	3.8510E-02
4.2942E-02	9.0035E-02	1.4209E-01	1.9649E-01	2.4933E-01	2.9721E-01
3.3797E-01	3.7065E-01	3.9521E-01	4.1217E-01	4.2677E-01	4.2209E-01
4.0517E-01	3.8145E-01	3.5477E-01	2.3525E-01	1.6536E-01	1.2671E-01
1.0317E-01	7.5820E-02	6.0157E-02	4.9918E-02	4.2680E-02	3.7285E-02
3.3106E-02	2.9773E-02	2.3792E-02			
7.5000E-01					
3.2071E-04	6.4142E-04	9.6213E-04	1.2828E-03	1.6036E-03	1.9243E-03
2.2450E-03	2.5658E-03	2.8865E-03	3.2073E-03	6.4158E-03	9.6266E-03
1.2841E-02	1.6060E-02	1.9285E-02	2.2517E-02	2.5757E-02	2.9006E-02
3.2264E-02	6.5532E-02	1.0014E-01	1.3551E-01	1.7038E-01	2.0325E-01
2.3279E-01	2.5806E-01	2.7858E-01	2.9424E-01	3.1200E-01	3.1482E-01
3.0705E-01	2.9265E-01	2.7468E-01	1.8525E-01	1.2993E-01	9.9167E-02
8.0542E-02	5.9064E-02	4.6823E-02	3.8838E-02	3.3199E-02	2.8998E-02
2.5746E-02	2.3152E-02	1.8498E-02			
1.0000E+00					
2.2778E-04	4.5558E-04	6.8336E-04	9.1115E-04	1.1389E-03	1.3667E-03
1.5945E-03	1.8223E-03	2.0501E-03	2.2779E-03	4.5561E-03	6.8347E-03
9.1141E-03	1.1394E-02	1.3676E-02	1.5959E-02	1.8244E-02	2.0530E-02
2.2818E-02	4.5838E-02	6.9092E-02	9.2358E-02	1.1517E-01	1.3691E-01
1.5695E-01	1.7474E-01	1.8991E-01	2.0223E-01	2.1834E-01	2.2422E-01
2.2210E-01	2.1442E-01	2.0333E-01	1.4020E-01	9.8277E-02	7.4710E-02
6.0513E-02	4.4270E-02	3.5065E-02	2.9072E-02	2.4845E-02	2.1698E-02
1.9262E-02	1.7320E-02	1.3836E-02			
1.5000E+00					
1.0422E-04	2.0844E-04	3.1266E-04	4.1687E-04	5.2109E-04	6.2531E-04
7.2953E-04	8.3374E-04	9.3796E-04	1.0422E-03	2.0843E-03	3.1264E-03
4.1683E-03	5.2100E-03	6.2515E-03	7.2928E-03	8.3337E-03	9.3743E-03
1.0414E-02	2.0782E-02	3.1040E-02	4.1102E-02	5.0856E-02	6.0165E-02
6.8884E-02	7.6871E-02	8.4003E-02	9.0186E-02	9.9499E-02	1.0476E-01
1.0641E-01	1.0513E-01	1.0173E-01	7.3999E-02	5.2109E-02	3.9332E-02
3.1674E-02	2.3051E-02	1.8223E-02	1.5095E-02	1.2893E-02	1.1256E-02
9.9905E-03	8.9818E-03	7.1737E-03			
2.0000E+00					
4.4639E-05	8.9277E-05	1.3392E-04	1.7855E-04	2.2319E-04	2.6783E-04
3.1247E-04	3.5711E-04	4.0174E-04	4.4638E-04	8.9273E-04	1.3390E-03
1.7852E-03	2.2312E-03	2.6771E-03	3.1228E-03	3.5683E-03	4.0135E-03
4.4584E-03	8.8835E-03	1.3241E-02	1.7493E-02	2.1600E-02	2.5522E-02
2.9215E-02	3.2640E-02	3.5760E-02	3.8543E-02	4.3020E-02	4.5994E-02
4.7528E-02	4.7797E-02	4.7041E-02	3.6207E-02	2.5802E-02	1.9379E-02

1.5516E-02	1.1228E-02	8.8578E-03	7.3302E-03	6.2576E-03	5.4613E-03
4.8461E-03	4.3561E-03	3.4784E-03			
3.5000E+00					
2.9736E-06	5.9471E-06	8.9207E-06	1.1894E-05	1.4868E-05	1.7841E-05
2.0815E-05	2.3788E-05	2.6762E-05	2.9735E-05	5.9468E-05	8.9197E-05
1.1892E-04	1.4863E-04	1.7834E-04	2.0803E-04	2.3770E-04	2.6736E-04
2.9699E-04	5.9182E-04	8.8232E-04	1.1664E-03	1.4420E-03	1.7072E-03
1.9603E-03	2.1994E-03	2.4232E-03	2.6302E-03	2.9904E-03	3.2741E-03
3.4800E-03	3.6102E-03	3.6706E-03	3.2557E-03	2.4672E-03	1.8574E-03
1.4666E-03	1.0415E-03	8.1605E-04	6.7323E-04	5.7375E-04	5.0022E-04
4.4356E-04	3.9852E-04	3.1799E-04			
5.0000E+00					
1.7780E-07	3.5560E-07	5.3340E-07	7.1120E-07	8.8900E-07	1.0668E-06
1.2446E-06	1.4224E-06	1.6002E-06	1.7780E-06	3.5559E-06	5.3335E-06
7.1109E-06	8.8878E-06	1.0664E-05	1.2440E-05	1.4215E-05	1.5989E-05
1.7762E-05	3.5418E-05	5.2863E-05	6.9994E-05	8.6712E-05	1.0292E-04
1.1854E-04	1.3347E-04	1.4766E-04	1.6102E-04	1.8508E-04	2.0530E-04
2.2151E-04	2.3368E-04	2.4193E-04	2.3614E-04	1.9155E-04	1.4759E-04
1.1608E-04	8.0969E-05	6.2926E-05	5.1737E-05	4.4013E-05	3.8331E-05
3.3965E-05	3.0501E-05	2.4319E-05			
7.5000E+00					
1.4729E-09	2.9459E-09	4.4188E-09	5.8917E-09	7.3646E-09	8.8376E-09
1.0310E-08	1.1783E-08	1.3256E-08	1.4729E-08	2.9458E-08	4.4185E-08
5.8910E-08	7.3633E-08	8.8352E-08	1.0307E-07	1.1778E-07	1.3248E-07
1.4718E-07	2.9372E-07	4.3895E-07	5.8224E-07	7.2299E-07	8.6058E-07
9.9446E-07	1.1241E-06	1.2490E-06	1.3686E-06	1.5908E-06	1.7877E-06
1.9576E-06	2.0993E-06	2.2124E-06	2.3888E-06	2.1259E-06	1.7304E-06
1.3816E-06	9.4617E-07	7.2403E-07	5.9132E-07	5.0140E-07	4.3584E-07
3.8572E-07	3.4609E-07	2.7560E-07			
1.0000E+01					
1.1483E-11	2.2965E-11	3.4447E-11	4.5930E-11	5.7412E-11	6.8895E-11
8.0377E-11	9.1859E-11	1.0334E-10	1.1482E-10	2.2964E-10	3.4446E-10
4.5926E-10	5.7404E-10	6.8880E-10	8.0354E-10	9.1826E-10	1.0329E-09
1.1476E-09	2.2911E-09	3.4267E-09	4.5504E-09	5.6583E-09	6.7467E-09
7.8120E-09	8.8509E-09	9.8600E-09	1.0836E-08	1.2679E-08	1.4361E-08
1.5865E-08	1.7181E-08	1.8302E-08	2.1049E-08	2.0028E-08	1.7190E-08
1.4124E-08	9.6835E-09	7.2997E-09	5.9143E-09	4.9961E-09	4.3338E-09
3.8305E-09	3.4338E-09	2.7310E-09			